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Specific features of the substitution of Fe3+ impurity ions for Zr4+ in NaZr2(PO4)3 single crystals

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Abstract

The EPR spectra of Fe3+ impurity ions in NaZr 2(PO4)3 single crystals at 300 K are investigated, and the spin Hamiltonian of these ions is determined. A comparative analysis of the spin-Hamiltonian and crystal-field tensors is performed using the maximum invariant component method. It is demonstrated that Fe3+ impurity ions substitute for Zr4+ ions with local compensator ions located in cavities of the B type. It is revealed that the invariant of the spin-Hamiltonian tensor B4 and the crystal-field tensor V44 4 depend substantially on the mutual arrangement of ions in the first and second coordination spheres. The corresponding dependences are analyzed.

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